NLM Batch Update File Layout
Last Updated: October 23, 2002

This document contains acceptable layouts and other information for successfully adding data through the Batch Update program.

Batch Layout 1 – RN Hyphens
Batch Layout 2 – Superlist Hyphens
Batch Layout 3 – Superlist No Hyphens
Batch Layout 4 – Non-Zero Filled RNs with Hyphens
Batch Layout 5 – Non-Zero Filled RNs No Hyphens
Additional Information
Element Type Reference

Batch Layout 1 – RN Hyphens

Line 1 of File:

Starting Column	Ending Column	Field	Description
1	1	File Description	Description of file (i.e., FILEINSERT, FILEUPDATE)
21	80	XLO	The XLO that should be identified with the records in the file

Other Lines of File:

Starting Column	Ending Column	Field	Description
1	1	Type ID	'R' is for Registry Number
2	12	RN	RN for the record
13	14	Action	The action to be performed on this file. This field can be 'IN' for insert, 'DE' for delete, or 'UP' for update.
15	17	Element Type	The type of data to be entered (i.e., a synonym or a molecular formula). See valid element types below.
18	80	Data	Data to be entered and associated with the record under the appropriate element type.

Above Example:
Line 1: *'FILEINSERT' is the File Description*
            'NLM' is the XLO

Line 2: 'R' is the Type ID (i.e., Registry Number)
            '000077-50-9' is the RN for the record
            'IN' is the Action
            '610' is the Element Type
            '059-45-8' is the Data

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Batch Layout 2 – Superlist Hyphens

```
File   Edit   Format   Help
FILEUPDATE             NLM
S041194-00-7IN6142-Pyrrolidinone, 5-hydroxy-1-methyl-
S041194-00-7IN6165-Hydroxy-N-methyl-2-pyrrolidone
S041194-00-7IN608C5-H9-N-O2
S041194-00-7IN632DART
S041194-00-7IN640041194007
S041194-00-7IN2611194-00-7
S069235-50-3IN614Acriflavine, hydrochloride
S069235-50-3IN616Acriflavine dihydrochloride
```
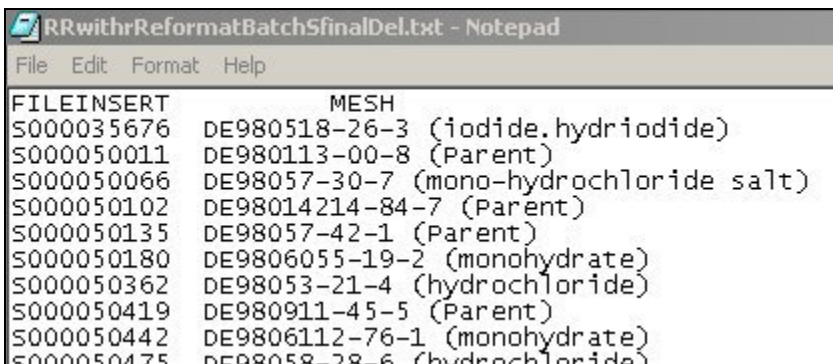
Line 1 of File:

Starting Column	Ending Column	Field	Description
1	1	File Description	Description of file (i.e., FILEINSERT, FILEUPDATE)
21	80	XLO	The XLO that should be identified with the records in the file

Other Lines of File:

Starting Column	Ending Column	Field	Description
1	1	Type ID	'S' is for Superlist ID
2	12	RN	RN for the record. Format is 11 digits with two hyphens. 041194-00-7 (The application will remove the hyphens to form the Superlist ID.)
13	14	Action	Action to be performed on this file. This field can be 'IN' for insert, 'DE' for delete, or 'UP' for update.
15	17	Element Type	The type of data to be entered (i.e., a synonym or a molecular formula). See valid element types below.
18	80	Data	Data to be entered and associated with the record under the appropriate element type.

• *Batch Layout 3 – Superlist No Hyphens*

```
RRwithrReformatBatchSfinalDel.txt - Notepad
File  Edit  Format  Help
FILEINSERT          MESH
S000035676  DE980518-26-3 (iodide.hydriodide)
S000050011  DE980113-00-8 (Parent)
S000050066  DE98057-30-7 (mono-hydrochloride salt)
S000050102  DE98014214-84-7 (Parent)
S000050135  DE98057-42-1 (Parent)
S000050180  DE9806055-19-2 (monohydrate)
S000050362  DE98053-21-4 (hydrochloride)
S000050419  DE980911-45-5 (Parent)
S000050442  DE9806112-76-1 (monohydrate)
S000050475  DE98058-28-6 (hydrochloride)
```

Line 1 of File:

Starting Column	Ending Column	Field	Description
1	1	File Description	Description of file (i.e., FILEINSERT, FILEUPDATE)
21	80	XLO	The XLO that should be identified with the records in the file

Other Lines of File:

Starting Column	Ending Column	Field	Description
1	1	Type ID	'S' is for Superlist ID
2	12	RN	RN for the record. Format 9 digits and 2 spaces. 000035676##
13	14	Action	Action to be performed on this file. This field can be 'IN' for insert, 'DE' for delete, or 'UP' for update.
15	17	Element Type	The type of data to be entered (i.e., a synonym or a molecular formula). See valid element types below.
18	80	Data	Data to be entered and associated with the record under the appropriate element type.

Batch Layout 4 – Non-Zero Filled RNs with Hyphens

```
File  Edit  Format  Help
FILEINSERT              TOXLINE
R87-31-0    DE290Diazo
R87-31-0    DE608B3-E2-N1
```

Line 1 of File:

Starting Column	Ending Column	Field	Description
1	1	File Description	Description of file (i.e., FILEINSERT, FILEUPDATE)
21	80	XLO	The XLO that should be identified with the records in the file

Other Lines of File:

Starting Column	Ending Column	Field	Description
1	1	Type ID	'R' is for Registry Number
2	12	RN	RN for the record. Format 7 digits with 2 hyphens and 4 spaces. 87-31-0####
13	14	Action	Action to be performed on this file. This field can be 'IN' for insert, 'DE' for delete, or 'UP' for update.
15	17	Element Type	The type of data to be entered (i.e., a synonym or a molecular formula). See valid element types below.
18	80	Data	Data to be entered and associated with the record under the appropriate element type.

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● *Batch Layout 5 – Non-Zero Filled RNs no Hyphens*

```
FILEINSERT            TOXLINE
R87310       IN290Diazo
R87310       IN608B3-E2-N1
```

Line 1 of File:

Starting Column	Ending Column	Field	Description
1	1	File Description	Description of file (i.e., FILEINSERT, FILEUPDATE)
21	80	XLO	The XLO that should be identified with the records in the file

Other Lines of File:

Starting Column	Ending Column	Field	Description
1	1	Type ID	'R' is for Registry Number
2	12	RN	RN for the record. Format 5 digits and 6 spaces. 87310######
13	14	Action	Action to be performed on this file. This field can be 'IN' for insert, 'DE' for delete, or 'UP' for update.
15	17	Element Type	The type of data to be entered (i.e., a synonym or a molecular formula). See valid element types below.
18	80	Data	Data to be entered and associated with the record under the appropriate element type.

Additional Information on the Batch Update program

- You may test a batch file in the Test environment by linking via the batch portal on **Toxnetdev**: http://toxnetdev.nlm.nih.gov:8100/dbmaint/
- You may run the batch file in the Production environment by linking via the batch portal on **Chem**: http://chem.sis.nlm.nih.gov:8080/dbmaint/chemidmaint.jsp

Element Type Reference

Element Name	Element Number	Element Name	Element Number
Note	211	Generic Name	920
MeSH Heading	251	Superlist Classification Code	950
CAS Registry Number	261	NIOSH Health Hazard	951
Name of Substance	290	Superlist Note	975
Molecular Formula Fragments	293	Related Registry Number	980
Mixture Name	294	Results Name	996
Classification Code	386	Internet Locators	999
Superlist Locator	403	Melting Point	1001
Molecular Formula	608	Boiling Point	1002
Other Registry Number	610	Water Solubility	1003
System Generated Number	611	log P (octanol-water)	1004
Systematic Name	614	Henry's Law Constant	1005
Synonyms	616	Atmospheric OH Rate Constant	1006
File Locator	632	pKa Dissociation Constant	1007
ID Number	640	Vapor Pressure	1008
Superlist Name	900		